



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:54 AM GMT

PDB ID : 1MSS  
Title : LARGE SCALE STRUCTURAL REARRANGEMENTS OF THE FRONT  
LOOPS IN MONOMERISED TRIOSEPHOSPHATE ISOMERASE, AS DE-  
DUCED FROM THE COMPARISON OF THE STRUCTURAL PROPER-  
TIES OF MONOTIM AND ITS POINT MUTATION VARIANT MONOSS  
Authors : Radha Kishan, K.V.; Wierenga, R.K.  
Deposited on : 1994-07-27  
Resolution : 2.40 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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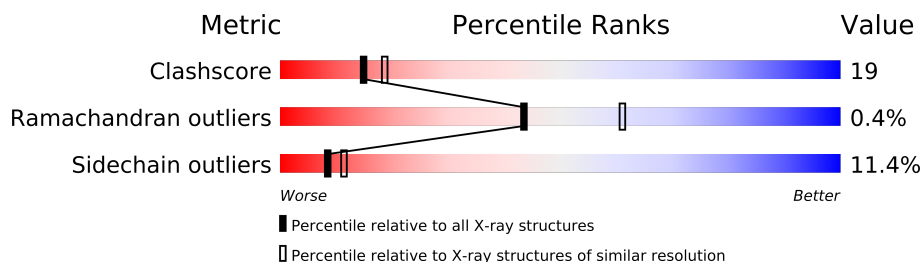
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	243	
1	B	243	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3698 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1821	1149	324	344	4			
1	B	242	Total	C	N	O	S	0	0	0
			1821	1149	324	344	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	SER	PHE	ENGINEERED	UNP P04789
A	46	SER	VAL	ENGINEERED	UNP P04789
A	68	GLY	ILE	ENGINEERED	UNP P04789
A	69	ASN	ALA	ENGINEERED	UNP P04789
A	70	ALA	LYS	ENGINEERED	UNP P04789
A	71	ASP	SER	ENGINEERED	UNP P04789
A	72	ALA	GLY	ENGINEERED	UNP P04789
A	?	-	ALA	DELETION	UNP P04789
A	?	-	PHE	DELETION	UNP P04789
A	?	-	THR	DELETION	UNP P04789
A	?	-	GLU	DELETION	UNP P04789
A	?	-	VAL	DELETION	UNP P04789
A	?	-	SER	DELETION	UNP P04789
A	81	ALA	PRO	ENGINEERED	UNP P04789
A	82	SER	ILE	ENGINEERED	UNP P04789
B	45	SER	PHE	ENGINEERED	UNP P04789
B	46	SER	VAL	ENGINEERED	UNP P04789
B	68	GLY	ILE	ENGINEERED	UNP P04789
B	69	ASN	ALA	ENGINEERED	UNP P04789
B	70	ALA	LYS	ENGINEERED	UNP P04789
B	71	ASP	SER	ENGINEERED	UNP P04789
B	72	ALA	GLY	ENGINEERED	UNP P04789
B	?	-	ALA	DELETION	UNP P04789
B	?	-	PHE	DELETION	UNP P04789
B	?	-	THR	DELETION	UNP P04789

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	DELETION	UNP P04789
B	?	-	VAL	DELETION	UNP P04789
B	?	-	SER	DELETION	UNP P04789
B	81	ALA	PRO	ENGINEERED	UNP P04789
B	82	SER	ILE	ENGINEERED	UNP P04789

- Molecule 2 is water.

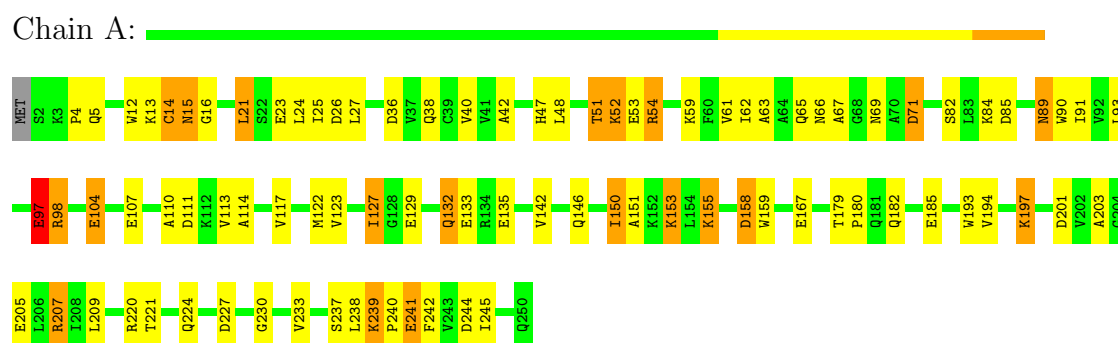
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	27	Total O 27 27	0	0
2	B	29	Total O 29 29	0	0

### 3 Residue-property plots

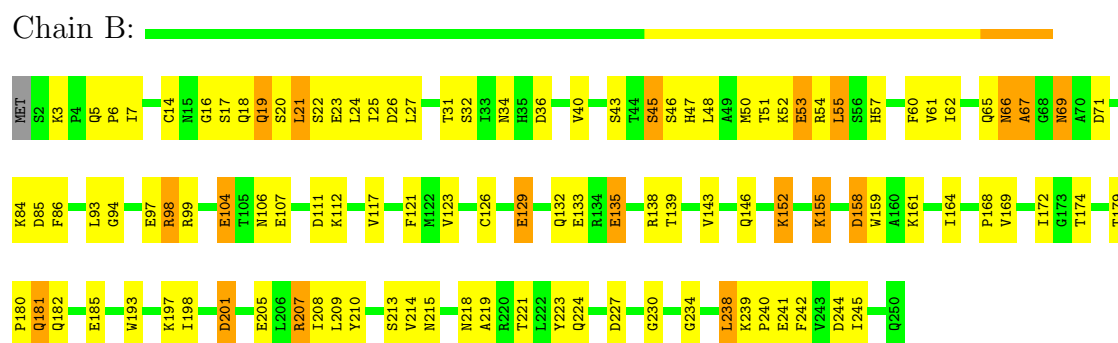
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: TRIOSEPHOSPHATE ISOMERASE



#### • Molecule 1: TRIOSEPHOSPHATE ISOMERASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.57Å 46.58Å 66.65Å 94.47° 69.82° 75.83°	Depositor
Resolution (Å)	24.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (24.00-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, $R_{free}$	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3698	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.84	12/1852 (0.6%)	0.84	18/2511 (0.7%)
1	B	0.80	11/1852 (0.6%)	0.85	18/2511 (0.7%)
All	All	0.82	23/3704 (0.6%)	0.85	36/5022 (0.7%)

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	CYS	C-O	6.37	1.35	1.23
1	A	104	GLU	CD-OE2	6.00	1.32	1.25
1	A	135	GLU	CD-OE2	5.94	1.32	1.25
1	B	205	GLU	CD-OE1	5.93	1.32	1.25
1	A	167	GLU	CD-OE1	5.92	1.32	1.25

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	A	227	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	B	111	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	244	ASP	CB-CG-OD1	-6.27	112.66	118.30
1	B	158	ASP	CB-CG-OD2	-6.25	112.68	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1821	0	1840	66	0
1	B	1821	0	1840	77	0
2	A	27	0	0	1	0
2	B	29	0	0	0	0
All	All	3698	0	3680	140	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

The worst 5 of 140 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:110:ALA:HB1	1:A:153:LYS:HD2	1.54	0.89
1:B:179:THR:H	1:B:182:GLN:NE2	1.77	0.83
1:B:179:THR:H	1:B:182:GLN:HE21	1.26	0.82
1:B:66:ASN:HD21	1:B:98:ARG:HD2	1.44	0.81
1:A:84:LYS:HE2	1:A:89:ASN:HB3	1.64	0.78

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/243 (99%)	228 (95%)	11 (5%)	1 (0%)	43	61
1	B	240/243 (99%)	229 (95%)	10 (4%)	1 (0%)	43	61
All	All	480/486 (99%)	457 (95%)	21 (4%)	2 (0%)	43	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	B	67	ALA



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/190 (99%)	167 (89%)	21 (11%)	9	12
1	B	188/190 (99%)	166 (88%)	22 (12%)	8	10
All	All	376/380 (99%)	333 (89%)	43 (11%)	8	11

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	LYS
1	B	27	LEU
1	B	213	SER
1	A	241	GLU
1	B	19	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	182	GLN
1	B	106	ASN
1	A	66	ASN
1	B	89	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.